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# Forces from highly focused laser beams: modeling, measurement and application to refractive index measurements

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**Abstract**

The optical forces in optical tweezers can be robustly modeled over a broad range of parameters using generalsed Lorenz–Mie theory. We describe the procedure, and show how the combination of experimental measurement of properties of the trap coupled with computational modeling, can allow unknown parameters of the particle—in this case, the refractive index—to be determined.

## Introduction

Light carries momentum, and changes in momentum equal applied forces. Focusing laser beams to small spot sizes creates high intensities and makes the momentum carried by the light comparable to other the other forces acting at that scale. The momentum can thus be exploited for applications ranging from atom trapping for Bose–Einstein condensation to molecule and nano-particle trapping to the trapping of entire live cells. The interaction of light with small and large particles is relatively easy to describe with Rayleigh scattering and geometrical optics, respectively. For the important particle size range with radii from 0.1 to 5 times the laser wavelength, direct solution of either the Maxwell equations or the vector Helmholtz equation is required. For the case of a spherical particle, an analytical solution is available: Lorenz–Mie theory (Lorenz 1890; Mie 1908).

We show how forces on particles in laser traps can be robustly modeled for a wide range of parameters by employing generalised Lorenz–Mie theory. We present results in the form of parameter landscapes which are of interest for a broader audience.

We compare computational modeling with experimental measurement of the forces acting in an optical trap, finding excellent agree between precision measurements of the optical spring constant and the theoretical predictions. We use the combination of such measurements and theoretical modeling to determine the refractive index of a microparticle.

# Computational Modeling of Optical Tweezers

A general divergence-free solution of the vector Helmholtz equation can be written in terms of vector spherical wavefunctions:

$$\begin{aligned}\mathbf{M}_{nm}^{(1,2)}(k\mathbf{r}) &= N_n h_n^{(1,2)}(kr)\mathbf{C}_{nm}(\theta,\phi) \\ \mathbf{N}_{nm}^{(1,2)}(k\mathbf{r}) &= \frac{h_n^{(1,2)}(kr)}{krN_n}\mathbf{P}_{nm}(\theta,\phi) + N_n\left(h_{n-1}^{(1,2)}(kr) - \frac{nh_n^{(1,2)}(kr)}{kr}\right)\mathbf{B}_{nm}(\theta,\phi)\end{aligned} \tag{1}$$

where $h_n^{(1,2)}(kr)$ are spherical Hankel functions of the first and second kind, $N_n = [n(n+1)]^{-1/2}$ are normalization constants, and $\mathbf{B}_{nm}(\theta,\phi) = \mathbf{r}\nabla Y_n^m(\theta,\phi)$, $\mathbf{C}_{nm}(\theta,\phi) = \nabla \times (\mathbf{r}Y_n^m(\theta,\phi))$, and $\mathbf{P}_{nm}(\theta,\phi) = \hat{\mathbf{r}}Y_n^m(\theta,\phi)$ are the vector spherical harmonics (Mishchenko 1991), and $Y_n^m(\theta,\phi)$ are normalized scalar spherical harmonics. The usual polar spherical coordinates are used, where $\theta$ is the co-latitude measured from the $+z$ axis, and $\phi$ is the azimuth, measured from the $+x$ axis towards the $+y$ axis.

In general, there will be an incoming part of the field:

$$\mathbf{E}_{\text{in}} = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} a_{nm}\mathbf{M}_{nm}^{(2)}(k\mathbf{r}) + b_{nm}\mathbf{N}_{nm}^{(2)}(k\mathbf{r}), \tag{2}$$

and an outgoing part:

$$\mathbf{E}_{\text{out}} = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} p_{nm}\mathbf{M}_{nm}^{(1)}(k\mathbf{r}) + q_{nm}\mathbf{N}_{nm}^{(1)}(k\mathbf{r}). \tag{3}$$

The fields can be compactly described by arranged the mode amplitude coefficients $a_{nm}$ and $b_{nm}$ as components of an incoming amplitude vector $\mathbf{a} = [a_{0,-1}, a_{0,0}, a_{0,+1}, .., b_{0,-1}, b_{0,0}, b_{0,+1}, ..]$, and $p_{nm}$ and $q_{nm}$ as an outgoing amplitude vector $\mathbf{p}$. If the electromagnetic properties of the scatterer are linear, these two will be related by a linear transformation

$$\mathbf{p} = \mathbf{T}\mathbf{a}. \tag{4}$$

Here, the matrix $\mathbf{T}$ is called the *transition matrix* or $T$-matrix. In principle, the field expansions and the $T$-matrix are infinite, but, in practice, can safely be truncated at a finite $n_{\max}$, typically with $n_{\max} \approx kr_0$, where $r_0$ is a radius that enclosed the particle or the beam waist.

When the particle is a homogeneous isotropic sphere, the $T$-matrix is diagonal, with elements given by the analytical Lorenz–Mie solution (Lorenz 1890; Mie 1908; van de Hulst 1981). For non-spherical particles, the $T$-matrix can still be calculated, but is a more computationally intensive task (Nieminen *et al.* 2003b).

The $T$-matrix need only be calculated once for each particle. It is a complete description of the scattering properties of the particle at that wavelength, with all information about the incident field contained in $\mathbf{a}$. If $\mathbf{a}$ and the $T$-matrix are known, then $\mathbf{p}$ can be found. At this point, the fields outside the particle are known, and can be used to find the momentum and angular momentum fluxes of the incoming and outgoing fields, with the optical force and torque being given by the differences between them. While one might guess that this would require numerical integration of the Poynting vector over a surface enclosing the particle, the orthogonality properties of the spherical functions involved can be used to reduce this to a sum of products of the mode amplitudes (Farsund and Felderhof 1996; Crichton and Marston 2000).

Finally, we need to consider how the incident field mode amplitudes can be found. This is a far from simple task; our method is to use an overdetermined point-matching algorithm in the far field (Nieminen *et al.* 2003a). This is most simply done in a coordinate system with the origin at the focus and the beam axis coincident with the $z$-axis, in which case the rotation symmetry of the beam can be used to greatly

reduce the computational requirements. An example of the instantaneous fields of a beam calculated in this manner is shown in figure 1.

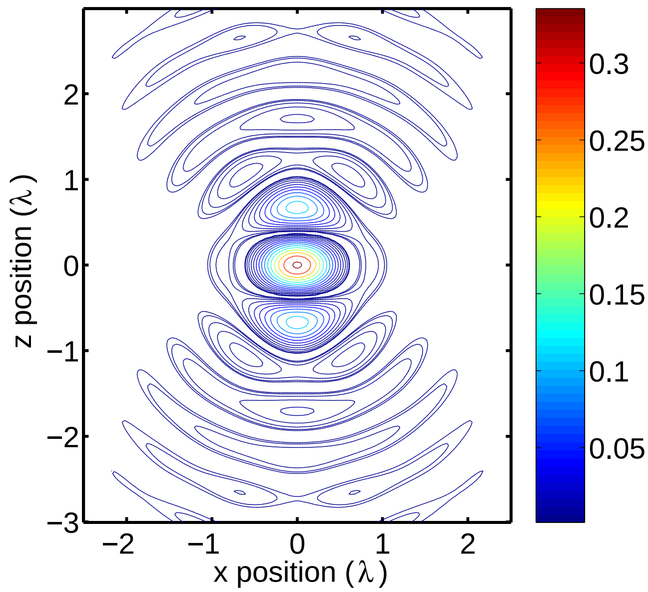


**Figure 1. Instantaneous fields of a tightly focused beam**

The mode amplitude coefficients of the beam in other coordinate systems can be found using the translation and rotation addition theorems for vector spherical wavefunctions (Choi *et al.* 1999; Videen 2000; Gumerov and Duraiswami 2003).

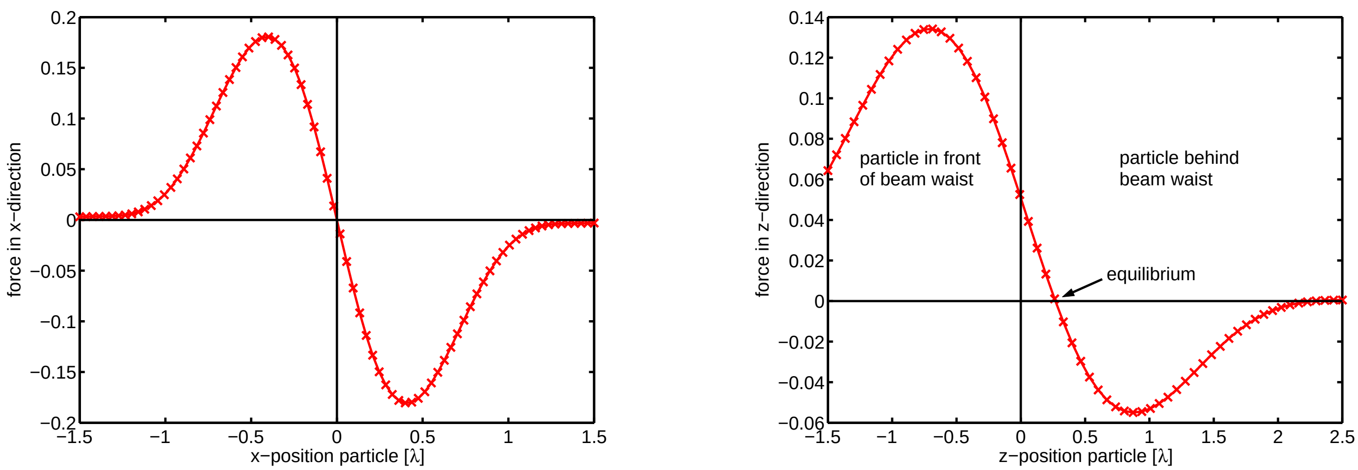


**Figure 2. Typical force curves**

The typical behaviour of the optical force as a function of radial and axial position within the trap is shown in figure 2. The radial force is symmetric about the beam axis, while the axial force is asymmetric about the focal plane; the gradient force acts towards the focal plane for displacements in either direction, while forces due to reflection of the trapping beam from the particle always act in the direction of propagation. Thus, the equilibrium position of the particle is somewhat past the focus. If the reflection force (ie, the force usually called the "scattering force", although it should be recognised that both this force *and* the gradient force arise through scattering) exceeds the maximum gradient force, trapping will not be possible. This will occur for high refractive index particles. The maximum axial restoring force can be calculated, and the

parameters for which particles can be trapped can be determined. Figure 3 shows the combinations of size and refractive index for which particles can be trapped.

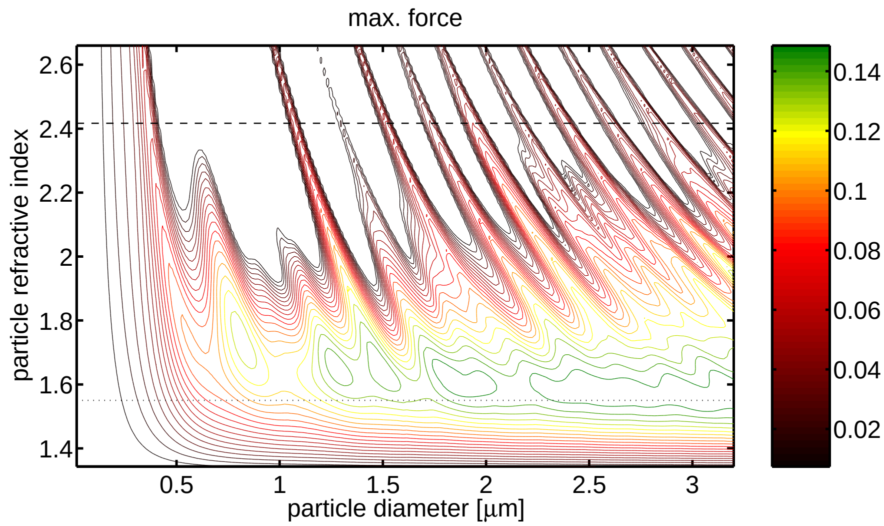


**FIgure 3. Maximum axial restoring force.** Where contours are absent, the reflection force overcomes the gradient force, and trapping is not possible.

## Comparison with Experiment and Refractive Index Measurement

Precision measurement of the properties of an optical trap allows the above modeling methodology to be tested. The spring constant of the trap was measured for a range of microspheres (silica, PMMA, and polystyrene). The silica microspheres were used to determine the laser power at the focus of the trap, and this power was then used to calculate the spring constants for the other microspheres as a function of refractive index. This is shown in figure 4. Excellent agreement was obtained between the refractive indices as indicated by comparison of the measured spring constants and the theoretical curves, and the known refractive indices .

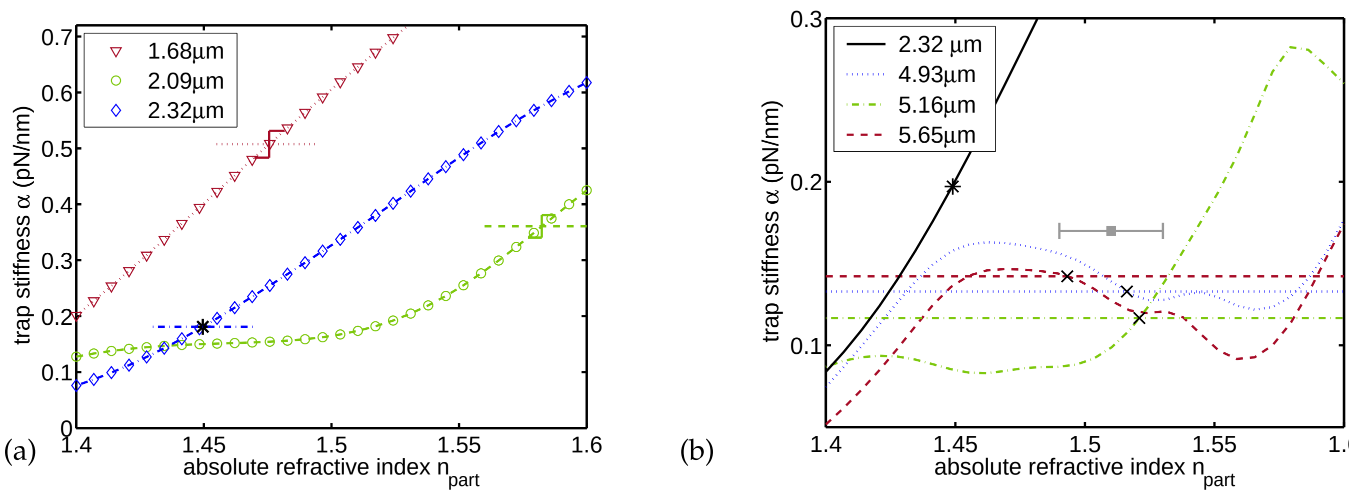


**Figure 4. Spring constants—measurement and calculation.** (a) shows calculated spring constants and experimental measurements for three different types of microspheres: silica (red), PMMA (blue), and polystyrene (green). (b) shows a calibration curve for a known microsphere (silica; black) and calculated

and measured spring constants for organosilica microspheres of unknown refractive index.

The refractive index of micrometre sized objects is an important quantity, strongly affecting their optical properties. However, it is not easily measured, especially for particles for which there is no equivalent bulk material, or which must remain in a particular environment to avoid alteration of optical properties, ruling out the possibility of index matching. Most methods based on scattering require a monodisperse sample—since the method presented here uses only a single particle at a time, a polydisperse sample presents no undue difficulty, and can even be an advantage, as some sizes in the range present may allow more accurate determination of the refractive index. Also, as a single-particle method, there is no need to account for complications such as multiple scattering. Our method of testing the accuracy of the modeling can be directly applied to the measurement of the refractive index of particles for which it is unknown. Accordingly, we measured the spring constants for different sizes of organosilica particles, and determined the refractive index to be $1.51 \pm 0.02$ (Knöner 2006).

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